OTAVA chemicals

Compounds for HTS
Chemical building blocks
Fragment libraries
Targeted libraries
Drug discovery services

HCN CHANNEL
BLOCKER LIBRARY

OTAVACHEMICALS.COM

OTAVA chemicals

OTAVA offers Hyperpolarization-Activated Cyclic Nucleotide-Gated (HCN) Channel Blocker library. This library provides an excellent basis for antianginal, antiarrhythmic, neuropathic research and drug discovery projects.

The library consists of **636 compounds***.

All compounds are:

- **in stock**; available amounts: 1 – 50 mg
- reactive, pan-assay interference (PAINS), redox-active and aggregator compounds were removed from the library.

QA/QC passed:

- minimal purity of compounds is **90%**;
- by **NMR** and/or **GC/LC/MS**
- **NMR spectra are available** upon request

Frendly packing services:

- **Cherry-picking is available**
- Supplied as dry powder or DMSO solution**
- Packaging in deep-well plates or barcoded vials***
- **Weighing out is free**

*Please note that the library does not contain known inhibitors. The compounds were selected with computational approach and are intended for screening projects

**there is additional fee for preparation of the solution

***4 ml amber glass vials or Deep-well plates: Matrix cat# 4247 (1.4 mL, Blank, Polypropylene, Round Bottom Tubes) w/CapMats. Or plates and vials provided by customer.

Design speciality:

Hyperpolarization-Activated Cyclic Nucleotide-Gated (HCN) Channel Blocker library was designed as a special screening library containing compounds with predicted HCN channels blocking activity and selectivity. The compounds have been selected by pharmacophore screening (see Appendix 1) of **OTAVAchemicals's Drug-like Green Collection** against two ligand-based pharmacophore models. The models were built based on known HCN channel blockers.

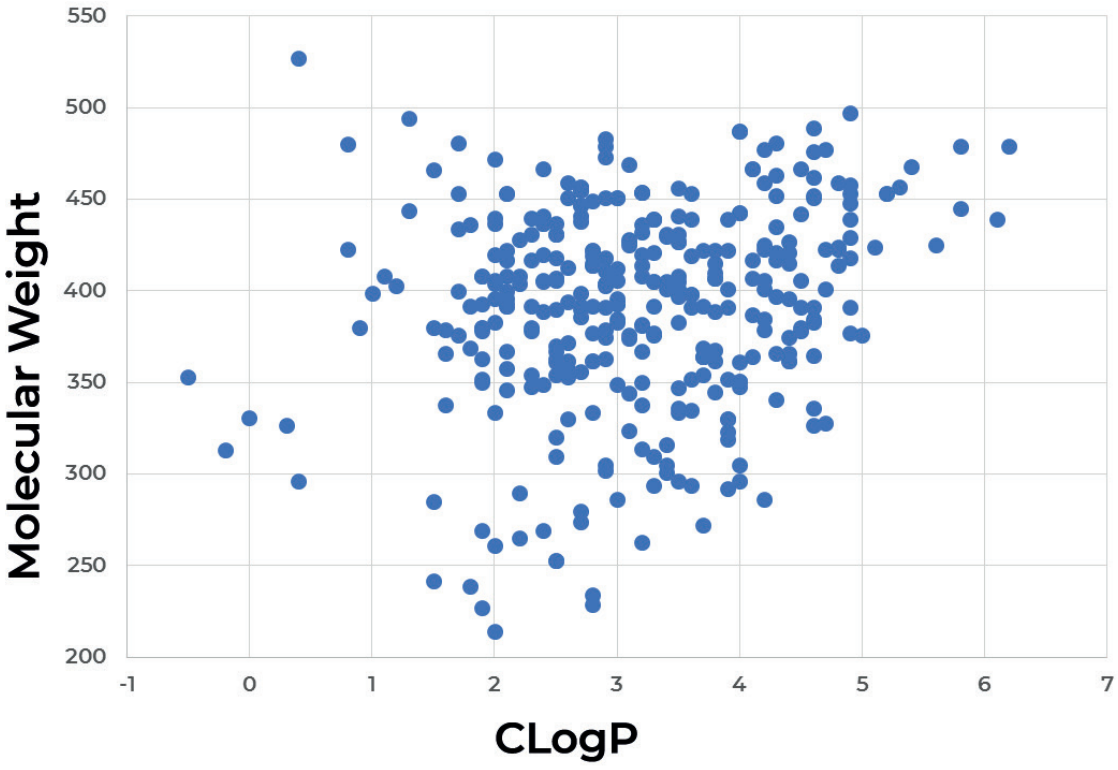
The summary of the library characteristics:

	Minimum	Maximum	Average value
Molecular Weight	213.3	527	387.7
Number of Hydrogen Bond Donors	0	4	0.7
Number of Hydrogen Bond Aceptors	2	10	4.6
Number of Rotatable Bonds	1	9	4.6
CLogP	-0.5	6.4	3.1
Number of Rings	2	6	3.9
Polar Surface Area	24.4	153.6	73

Distribution of physicochemical properties of compounds in the library:

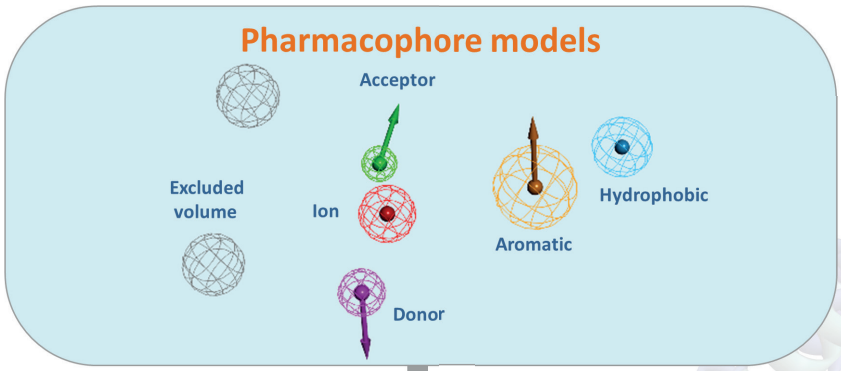
93% Drug-like

41% Lead-like



Appendix 1

Scheme 1. Application of ligand-based pharmacophore modeling for targeted library:



Literature review, carefully selecting of compounds to training set

Selection of important molecular descriptors

Development of pharmacophore models

- Validation, optimization and selection of the best models
- Pharmacophore screening
- Weighted rescoring + Rescoring based on molecular descriptors (QSAR)
- Selection of the top-scored compounds

Screening collection

Visual analysis

Results

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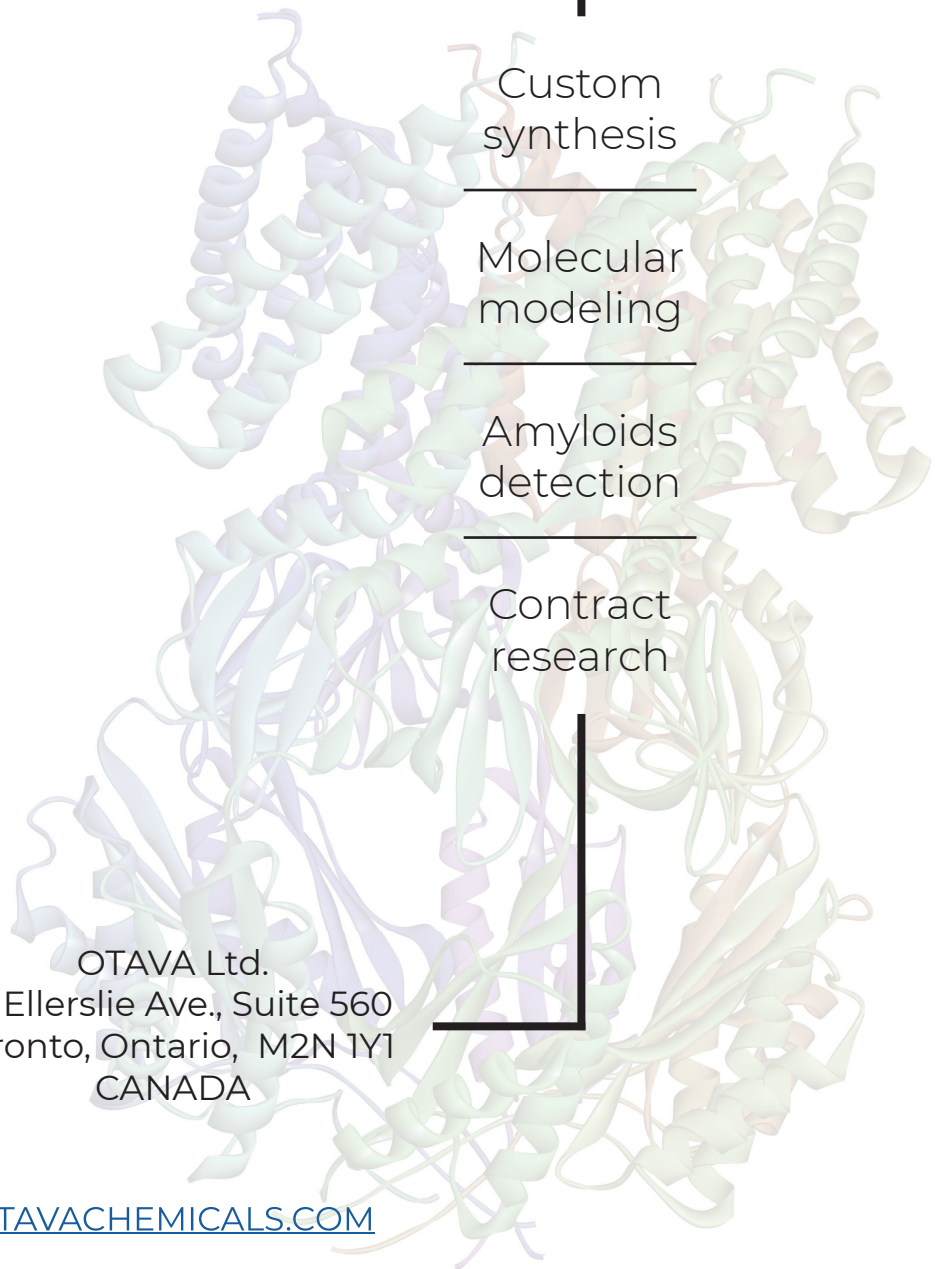

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